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Percolation transition in two dimensional electron gas: A cellular automaton model

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ABSTRACT

Using the notion of phase coherence length ζ_ϕ, a quantum cellular automaton model for two-dimensional electron gas (2DEG) is designed leading to a new type of disorder-driven electronic percolation transition. This transition is shown to be accompanied by a metal-insulator transition, as well as a singularity in the electronic compressibility. The cellular automaton model for transporting the electrons is developed in terms of the temperature (T) and the disorder strength (Δ). At the transition line some power-law behaviors emerge with critical exponents consistent with the Gaussian free field (GFF) and partly the percolation theory. Our model yields the important features of the experimental observations, e.g. the singularity in the conductivity in a critical density and also the universality (non-universality) of the metal-insulator transition (MIT) for the small (large) disorders in 2DEG. A $T-\Delta$ phase diagram of the electron gas is drawn in which in addition to the mentioned transition line, a zero-heat capacity line is also observed in which the system becomes unstable.

Many classical and quantum systems have the potential to be described in terms of the percolation theory in some limits [1]. Despite its very simple rules, this theory has successfully been applied to describe a large variety of natural [1], social [2], and quantum [3,4] systems. The description of insulating-non-insulating phase transitions in terms of the percolation theory has been done in some systems, like quantum Hall effect systems [3] and metal-insulator transition (MIT) in 2DEG [4]. In the latter case, in an essentially classical scheme, it was claimed that the disorder-induced *valleys and mountains* created by unscreened coulomb potential at low densities [4] is responsible for the experimentally observed MIT in 2DEG [5,6]. This approach due to its generality and simpleness sounds very promising in quantum systems. The percolation theory, when is mixed by the cellular automaton models, has proved to be very powerful in describing the natural systems [7]. The classical example is the sandpiles on the percolation lattices which has some relations with the propagation of fluid in the reservoirs [8]. The easiest way to generalize this concept to the quantum systems is to use the notion of phase-relaxation length ζ_ϕ above which the electronic transport is classical, i.e. the system can be meshed by means of ζ_ϕ. A cellular automaton model can therefore be designed for the transport of electrons with spatial scales below and above ζ_ϕ. Consider for example a highly biased metal-oxide-semiconductor (MOS) junction with an inversion layer in which a 2D electron gas is formed whose density is controlled by the bias voltage [6]. In this system the metal and semiconductor have the role of electronic reservoirs from which the electrons can be transferred to the inversion layer, i.e. 2DEG and vice versa. The localization of electrons in such a system is roughly controlled by ζ_ϕ. In Fig. 1(left) this system has schematically been shown, in which the 2DEG has been meshed by some cells (hexagons) of the linear scale ζ_ϕ. The aim of the present paper is to develop a cellular automaton model with local transition rules based on the local chemical potential. The electrons, when transmitted from the electronic reservoirs to the inversion layer, respect to some simple automaton rules for traveling to the neighboring cells, resulting to a chain of in-plane transmissions. By coloring the cells in which a transmission has occurred, a colored area results. A spanning colored area means that some electrons have traveled throughout the 2D sample and contributed to the in-plane conductivity. This method, when compared with the other percolation methods, e.g. two-component effective medium theory [4], is proved to be very rich and powerful. Our main observation of the paper, namely that in the vanishing inter-particle interaction, and in the diffusive phase the system experiences a transition from the localized states (in which the electrons cannot travel throughout the sample) to the extended states (metallic states in the sense that the conductivity is a decreasing function of the temperature), shows that the system can have a MIT which is not interaction-driven (like Wigner-Mott systems [9–11]), nor Anderson-localization type [12–14] (stating that the in plane magnetic field that destroys the metallic phase), instead a *finite temperature disorder-driven percolation transition* (for 2D MIT see Ref. [15]). We name this behavior as *semi-classical localization* of electrons.

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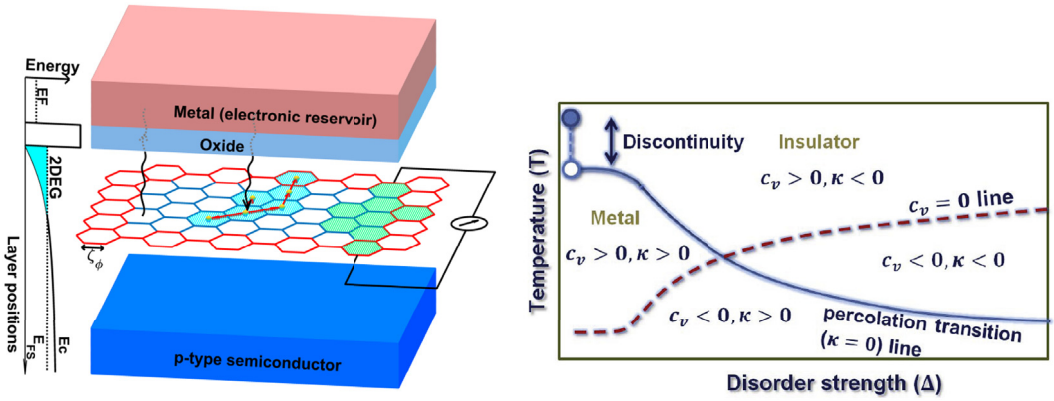

Fig. 1. (Left) A schematic representation of a MOS system with a 2DEG in the inversion layer. The 2DEG has been mashed by many artificial hexagons of the linear size ζ_ϕ. Shadowed area is composed of sites from which the electrons have passed. A spanning shadowed area contributes to the conductivity. (b) The total (schematic) $T-\Delta$ phase diagram with zero-κ (compressibility) (blue full line) and zero-c_v (red broken line). (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

The Fig. 1(right) shows our final $T-\Delta$ phase diagram. The full (blue) line shows the second order percolation transition above (under) which the system is localized (extended). The compressibility diverges at this line, signaling the instability of the system. The electron density as well as the chemical potential show also some singular behaviors at this line. In the extended phase, the conductivity has a decreasing behavior in terms of temperature which is the characteristics of the *metallic phase*. The dashed (red) line shows the zero-heat capacity ($C_v = 0$) line below which $C_v < 0$ in which the electron gas is unstable. The vertical full line shows that the system shows a discontinuity from $\Delta = 0$ to positive Δ values.

1. The method

When a quantum system is in the diffusive regime, the dynamics of electrons is divided to two scales relative to the phase relaxation length $\zeta_\phi \equiv \sqrt{D\tau_\phi}$ in which D is the diffusion coefficient and τ_ϕ is the phase relaxation time associated with inelastic or spin-flip scattering up to which the electrons retain their coherence, i.e. the quantum phase is maintained up to $t = \tau_\phi$. Therefore the spatial dynamics of the electrons is divided to two spatial (r) scales: $l \ll r \ll \zeta_\phi$ and $r \gg \zeta_\phi$ in which l is the mean free path due to the electron-electron or the electron-phonon interactions. For $r \gg \zeta_\phi$ the electron dynamics is semi-classical, since the quantum coherence becomes negligible and since the dynamics of a random phase particle is classical, one can use classical Boltzmann transport equation [17]. The existence of such a temperature dependent spatial scale is crucial in e.g. self-averaging of quantum systems [16]. In this approach one subdivides the system into many cells with the linear sizes $\Delta L \sim \zeta_\phi(T)$. The electron gas inside the cells should be treated quantum mechanically, whereas the transport between the cells is semi-classical. The cells should be considered most symmetric, i.e. circles in 2DEG which is estimated by hexagons in the present work. The meshed space has schematically drawn in Fig. 1 in contact with some electronic reservoirs (metal and semiconductor) from which the electrons can cross out. The electrons can enter the 2DEG from the metal by tunneling, or from the semiconductor directly which makes the neighboring cells excited and leads to electron transport to the other cells. The electrons which have traveled throughout the 2D sample, contribute to the in-plane conductivity. The local rules for these electron transmissions are according to the local free energy and the chemical potential of the cells. Actually one can think of this mapping (onto the classical percolation problem) as subdividing the main system to many (hexagonal) boxes with periodic boundary conditions, between which the electrons can pass. If one let the local chemical potentials of each of these boxes are equal and the electronic transitions between the boxes are quantum mechanical, then the effect of this meshing becomes trivial. We have assumed that the local chemical potentials are not the same (due to presence of charged disorder) and also the transition between the boxes is classical which are reasonable.

The energy of the electron gas and the chemical potential inside each cell is calculated by means of the Thomas-Fermi-Dirac (TFD) approach. The average energy of the ith cell, inside which the charge in supposed to be uniform, is $\langle E_i\rangle = K(T, \tilde{N}_i) + V_{ee}(T, \tilde{N}_i) + E_{\rm imp}(T, \tilde{N}_i)$ in which the terms are finite temperature averages of the kinetic, the electron-electron interaction and the impurity energies respectively and $\tilde{N}_i$ is the number of electrons in the cell. In the weak interaction limit (i.e. in which the dominant term is the kinetic energy) $K(T, \tilde{N}_i)$ is readily shown to be $-\frac{2mA\pi}{\beta^2\hbar^2}\mathrm{Li}_2(1-e^{\beta\epsilon_F^i})$ in which $\beta = 1/k_BT$, $\varepsilon_F^i = \frac{\hbar^2}{2\,\mathrm{m}}\left(\frac{\tilde{N}_i}{\pi A}\right)$, A is the area of the cell which is approximated by $\pi\zeta_\phi^2$, m is the electron mass and $\mathrm{Li}_2(z) \equiv \sum_{i=1}^{\infty}\frac{z^n}{2^n}$ is the poly logarithmic function. In this paper we consider free particles, i.e. $V_{ee} \equiv 0$ by which we show that the existence of the localized-extended phase transition in our system is not interaction-driven. The same arguments also hold for the impurity energy whose classical form is $E_{\rm imp} = -\mathrm{Arcsinh}(1)\frac{Ze^2}{\pi\varepsilon_0\zeta_\phi}\tilde{N}_i$ in which Ze is the electric charge of the impurity in the cell and the potential range and its corresponding integrals are supposed to be limited to the cell. The sum of the above mentioned contributions yields the total energy as $E_T = \sum_{i=1}^{L}[-\alpha T^2\mathrm{Li}_2(1-e^{N_i/T}) - \gamma_i N_i]$, in which $\alpha = 2\,\mathrm{m}\left(\frac{\pi k_B\zeta_\phi(T)}{\hbar}\right)^2$, $\gamma_i = \sinh^{-1}(1)\frac{\alpha e^2}{\pi\varepsilon_0 k_B\zeta_\phi(T)}Z_i$, $N_i = \frac{k_B}{\alpha}\tilde{N}_i$ and L is the total number of cells. This is a simplified theory which has the ability to show the non-trivial main features of the experiments, to be described in the following section.

The chemical potential of a cell ($\mu_i = \partial A_i/\partial N|_{V,T}$ in which A_i is the Helmholtz free energy of the ith cell) as the main building block of the transition rules of electrons between cells is obtained using the relation $A_{\tilde{N}}(V, T) - T\left(\frac{\partial A}{\partial T}\right)_{\tilde{N},V} = \langle E\rangle$. By considering the fact that $\mu(T\to 0)\to 0$ and $\zeta_\phi(T) = aT^{-1/2}$ for two dimensional electron gas [17] (a is a proportionality constant), the solution is obtained to be $\mu_i = k_BT\ln(e^{h_i} - 1) - IZ_iT^{\frac{1}{2}}$ in which $I = \sinh^{-1}(1)\frac{e^2}{\pi\varepsilon_0\sqrt{Da}}$, $h_i = \frac{N_i}{T}$ and i stands for the ith cell. The effect of randomness of Z_i's, which captures the on-site (diagonal) disorder is investigated. Z_i's are supposed to be random noise with a uniform probability measure $P(Z) = \frac{1}{\Delta}\Theta(\Delta/2 + (Z - Z_0))\Theta(\Delta/2 - (Z - Z_0))$ in which Δ shows the disorder strength, $Z_0 = \langle Z\rangle$ is the average of Z and Θ is the step function and $\langle Z_iZ_j\rangle = \delta_{ij}$ in which $\langle\ \rangle$ shows the ensemble average and δ is the Kronecker delta. The present model is a toy model which highlights the semi-classical aspects of the electronic transport in the absence of e-e interaction. In fact, considering the charged disorder for this free-electronic system is sufficient to represent a new-type disorder-driven